Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 05:48 PM EST

PDB ID	:	4FJY
Title	:	Crystal structure of PI3K-gamma in complex with quinoline-indoline inhibitor 24f
Authors	:	Whittington, D.A.; Tang, J.; Yakowec, P.
Deposited on	:	2012-06-12
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

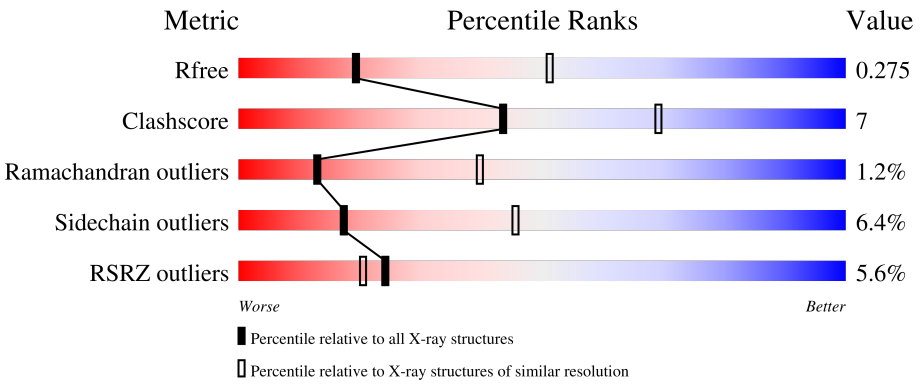
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	960	5% 69% 17% • 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6858 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

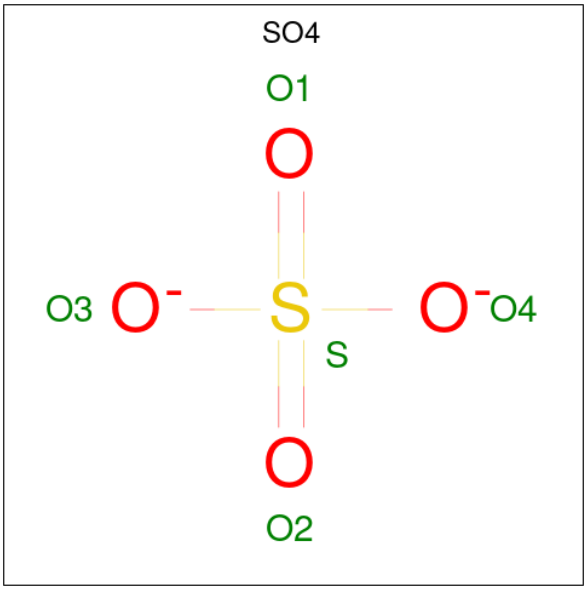
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	839	6795	4363	1158	1240	34	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLY	-	expression tag	UNP P48736

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

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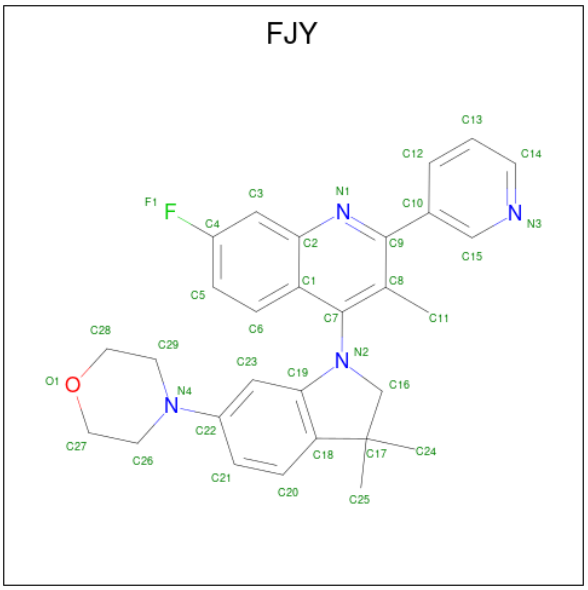
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is 4-[3,3-dimethyl-6-(morpholin-4-yl)-2,3-dihydro-1H-indol-1-yl]-7-fluoro-3-methyl-2-(pyridin-3-yl)quinoline (three-letter code: FJY) (formula: $C_{29}H_{29}FN_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	35	29	1	4	1	0	0

- Molecule 4 is water.

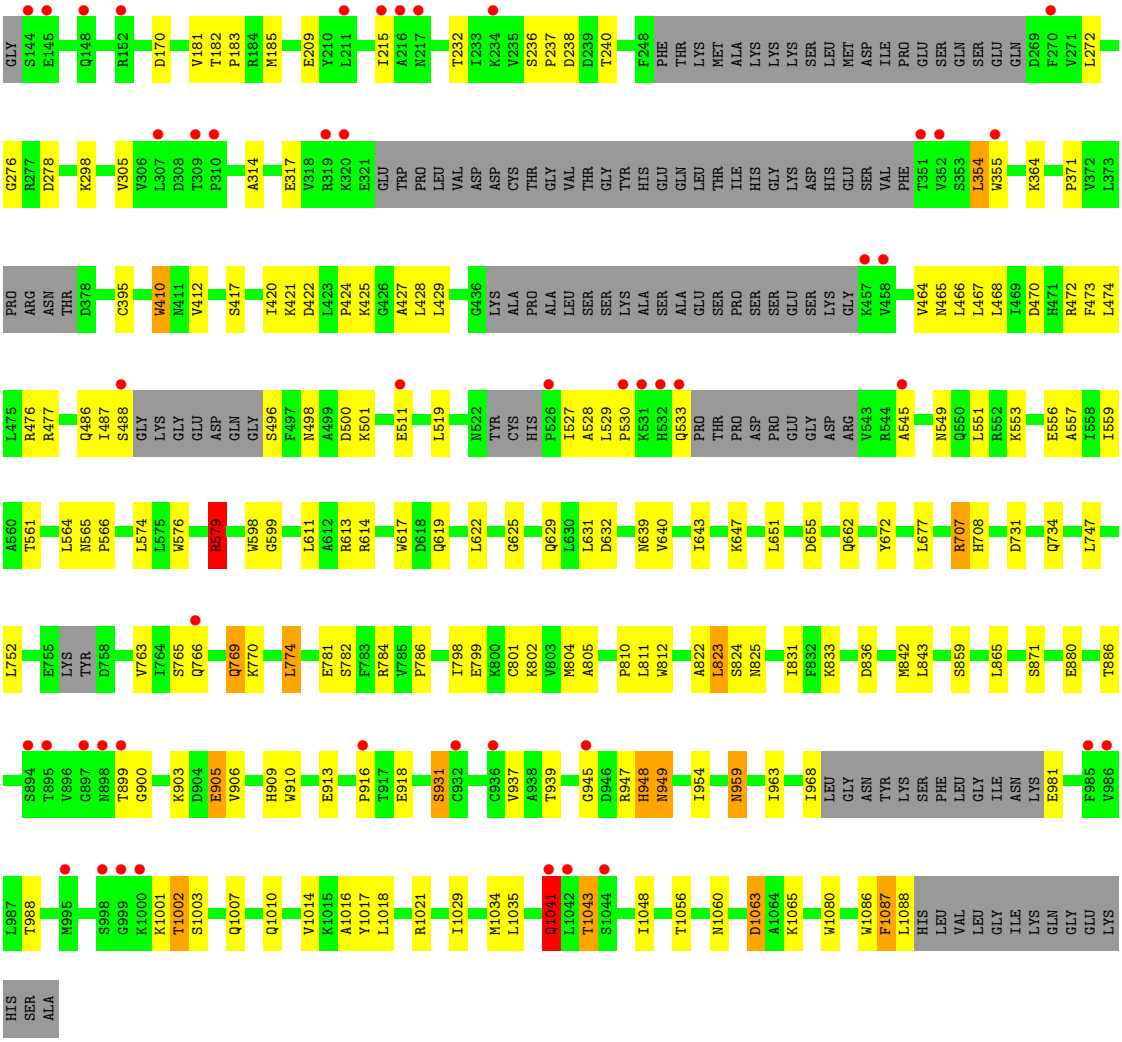
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	13	13	13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

Chain A: 5% 69% 17% • 13%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.22Å 67.71Å 106.77Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.90) 99.6 (29.73-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.275 0.195 , 0.275	Depositor DCC
R_{free} test set	1661 reflections (7.25%)	wwPDB-VP
Wilson B-factor (Å^2)	86.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6858	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FJY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.52	6/6938 (0.1%)	0.59	1/9384 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	918	GLU	CD-OE1	-7.47	1.17	1.25
1	A	918	GLU	CD-OE2	5.88	1.32	1.25
1	A	410	TRP	CD2-CE2	5.25	1.47	1.41
1	A	1080	TRP	CD2-CE2	5.15	1.47	1.41
1	A	617	TRP	CD2-CE2	5.07	1.47	1.41
1	A	1086	TRP	CD2-CE2	5.06	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	747	LEU	CA-CB-CG	5.24	127.36	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6795	0	6840	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	0	0	0
3	A	35	0	29	9	0
4	A	13	0	0	0	0
All	All	6858	0	6869	92	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.35	1.09
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.72	0.72
1:A:804:MET:HB2	3:A:1204:FJY:C4	2.20	0.70
1:A:272:LEU:HB3	1:A:305:VAL:HG21	1.74	0.69
1:A:948:HIS:CD2	1:A:948:HIS:N	2.62	0.68
1:A:948:HIS:CD2	1:A:948:HIS:H	2.12	0.66
1:A:810:PRO:HG2	3:A:1204:FJY:H24	1.78	0.66
1:A:556:GLU:HA	1:A:559:ILE:HD12	1.78	0.65
1:A:625:GLY:O	1:A:629:GLN:HG3	1.95	0.65
1:A:354:LEU:HD12	1:A:527:ILE:HG22	1.80	0.64
1:A:880:GLU:O	3:A:1204:FJY:H4	1.99	0.63
1:A:899:THR:HA	1:A:1087:PHE:HE2	1.62	0.63
1:A:842:MET:HE2	1:A:871:SER:HB3	1.81	0.62
1:A:629:GLN:HG2	1:A:1029:ILE:CG1	2.22	0.61
1:A:1018:LEU:HD23	1:A:1021:ARG:HD3	1.82	0.61
1:A:276:GLY:HA2	1:A:822:ALA:HB2	1.83	0.59
1:A:640:VAL:O	1:A:643:ILE:HG12	2.04	0.58
1:A:886:THR:OG1	3:A:1204:FJY:H28	2.03	0.58
1:A:843:LEU:HB3	1:A:1034:MET:HG3	1.86	0.57
3:A:1204:FJY:H23	3:A:1204:FJY:H16	1.87	0.57
1:A:810:PRO:HG2	3:A:1204:FJY:C5	2.34	0.56
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.87	0.56
1:A:802:LYS:HG3	1:A:812:TRP:HB3	1.87	0.56
1:A:954:ILE:HA	1:A:959:ASN:O	2.06	0.56
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.89	0.55
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.88	0.55
1:A:939:THR:HB	1:A:945:GLY:HA2	1.90	0.54
1:A:784:ARG:O	1:A:786:PRO:HD3	2.08	0.53
1:A:798:ILE:HD12	1:A:798:ILE:H	1.74	0.52
1:A:467:LEU:O	1:A:476:ARG:HD2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.92	0.51
1:A:272:LEU:HB3	1:A:305:VAL:CG2	2.41	0.51
1:A:1001:LYS:HG2	1:A:1002:THR:H	1.74	0.51
1:A:799:GLU:H	1:A:799:GLU:CD	2.15	0.50
1:A:948:HIS:N	1:A:948:HIS:HD2	2.08	0.50
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.47	0.50
1:A:631:LEU:HD22	1:A:677:LEU:HD22	1.94	0.49
1:A:425:LYS:HD2	1:A:473:PHE:CE2	2.48	0.49
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.48	0.49
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.93	0.49
1:A:899:THR:HA	1:A:1087:PHE:CE2	2.44	0.48
3:A:1204:FJY:H8	3:A:1204:FJY:H9	1.50	0.48
1:A:551:LEU:HD22	1:A:574:LEU:HD11	1.95	0.48
1:A:236:SER:O	1:A:238:ASP:N	2.46	0.48
1:A:474:LEU:HD23	1:A:528:ALA:HB2	1.95	0.48
1:A:613:ARG:O	1:A:613:ARG:CG	2.62	0.48
1:A:734:GLN:NE2	1:A:782:SER:O	2.46	0.48
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.96	0.48
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.49	0.48
1:A:707:ARG:HD3	1:A:707:ARG:H	1.79	0.47
1:A:1041:GLN:HB3	1:A:1043:THR:HG23	1.96	0.47
1:A:422:ASP:HB3	1:A:599:GLY:O	2.15	0.47
1:A:424:PRO:HG3	1:A:598:TRP:O	2.15	0.47
1:A:181:VAL:O	1:A:185:MET:HG2	2.15	0.47
1:A:549:ASN:O	1:A:553:LYS:HG2	2.14	0.46
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.97	0.46
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.96	0.46
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.97	0.46
1:A:1060:ASN:ND2	1:A:1063:ASP:HB2	2.31	0.46
1:A:557:ALA:O	1:A:561:THR:HG23	2.16	0.45
1:A:182:THR:HB	1:A:183:PRO:CD	2.45	0.45
1:A:801:CYS:HA	1:A:812:TRP:O	2.16	0.44
1:A:486:GLN:HG2	1:A:487:ILE:H	1.82	0.44
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.88	0.44
1:A:622:LEU:HD13	1:A:647:LYS:HB3	2.00	0.44
1:A:576:TRP:O	1:A:579:ARG:HD3	2.18	0.43
1:A:632:ASP:C	1:A:632:ASP:OD1	2.56	0.43
1:A:949:ASN:H	1:A:949:ASN:HD22	1.66	0.43
1:A:278:ASP:HB2	1:A:784:ARG:HH12	1.82	0.43
1:A:811:LEU:O	1:A:831:ILE:HA	2.19	0.43
1:A:937:VAL:HG21	1:A:1016:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:TRP:HA	1:A:913:GLU:HG2	2.01	0.43
1:A:424:PRO:HD2	1:A:427:ALA:HB2	2.00	0.43
1:A:639:ASN:O	1:A:643:ILE:HG23	2.19	0.43
1:A:903:LYS:HB3	1:A:906:VAL:HG23	2.01	0.43
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.48	0.42
1:A:314:ALA:O	1:A:317:GLU:HB2	2.19	0.42
1:A:765:SER:O	1:A:769:GLN:HB2	2.19	0.42
1:A:770:LYS:O	1:A:774:LEU:HB2	2.19	0.42
1:A:810:PRO:CG	3:A:1204:FJY:H24	2.47	0.42
1:A:947:ARG:NH2	1:A:963:ILE:O	2.53	0.42
1:A:371:PRO:HG2	1:A:511:GLU:O	2.19	0.42
1:A:182:THR:HB	1:A:183:PRO:HD3	2.02	0.42
1:A:611:LEU:O	1:A:614:ARG:HD3	2.20	0.42
1:A:931:SER:OG	1:A:959:ASN:ND2	2.53	0.41
1:A:355:TRP:HA	1:A:421:LYS:HB2	2.02	0.41
1:A:707:ARG:H	1:A:707:ARG:HH11	1.68	0.41
1:A:1007:GLN:HA	1:A:1010:GLN:HE21	1.84	0.41
1:A:804:MET:HB2	3:A:1204:FJY:C3	2.50	0.41
1:A:903:LYS:HE3	1:A:905:GLU:HB3	2.02	0.41
1:A:833:LYS:NZ	1:A:836:ASP:OD2	2.39	0.40
1:A:565:ASN:HA	1:A:566:PRO:HD2	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	819/960 (85%)	756 (92%)	53 (6%)	10 (1%)	13 40

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	900	GLY
1	A	1087	PHE
1	A	545	ALA
1	A	579	ARG
1	A	805	ALA
1	A	1041	GLN
1	A	823	LEU
1	A	237	PRO
1	A	1056	THR
1	A	916	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	755/857 (88%)	707 (94%)	48 (6%)	17 45

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ASP
1	A	215	ILE
1	A	232	THR
1	A	240	THR
1	A	298	LYS
1	A	354	LEU
1	A	395	CYS
1	A	417	SER
1	A	420	ILE
1	A	464	VAL
1	A	470	ASP
1	A	472	ARG
1	A	477	ARG
1	A	488	SER
1	A	496	SER
1	A	498	ASN
1	A	501	LYS

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Mol	Chain	Res	Type
1	A	533	GLN
1	A	579	ARG
1	A	619	GLN
1	A	662	GLN
1	A	707	ARG
1	A	731	ASP
1	A	752	LEU
1	A	763	VAL
1	A	766	GLN
1	A	769	GLN
1	A	774	LEU
1	A	781	GLU
1	A	823	LEU
1	A	824	SER
1	A	825	ASN
1	A	865	LEU
1	A	905	GLU
1	A	909	HIS
1	A	931	SER
1	A	948	HIS
1	A	949	ASN
1	A	959	ASN
1	A	968	ILE
1	A	981	GLU
1	A	988	THR
1	A	1002	THR
1	A	1003	SER
1	A	1041	GLN
1	A	1043	THR
1	A	1063	ASP
1	A	1088	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	391	GLN
1	A	459	GLN
1	A	498	ASN
1	A	601	GLN
1	A	639	ASN
1	A	734	GLN
1	A	743	GLN

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Mol	Chain	Res	Type
1	A	766	GLN
1	A	769	GLN
1	A	773	ASN
1	A	948	HIS
1	A	949	ASN
1	A	959	ASN
1	A	1007	GLN
1	A	1010	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1203	-	4,4,4	0.39	0	6,6,6	0.17	0
2	SO4	A	1202	-	4,4,4	0.36	0	6,6,6	0.15	0
3	FJY	A	1204	-	40,40,40	1.88	6 (15%)	54,60,60	2.33	18 (33%)
2	SO4	A	1201	-	4,4,4	0.35	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FJY	A	1204	-	-	1/12/35/35	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1204	FJY	C10-C9	-7.72	1.40	1.49
3	A	1204	FJY	C7-N2	-5.82	1.35	1.44
3	A	1204	FJY	C19-N2	-3.24	1.33	1.39
3	A	1204	FJY	C7-C1	-2.24	1.40	1.44
3	A	1204	FJY	C2-N1	-2.03	1.34	1.37
3	A	1204	FJY	C3-C4	2.02	1.39	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1204	FJY	O1-C28-C29	-7.74	94.74	111.80
3	A	1204	FJY	C23-C22-N4	-6.51	114.33	121.33
3	A	1204	FJY	C8-C7-N2	4.24	121.91	118.38
3	A	1204	FJY	C29-N4-C26	4.16	120.69	111.52
3	A	1204	FJY	C16-N2-C7	4.04	126.17	121.53
3	A	1204	FJY	C25-C17-C24	3.36	113.27	109.18
3	A	1204	FJY	C16-N2-C19	3.27	111.41	109.31
3	A	1204	FJY	C21-C22-N4	3.25	125.85	121.38
3	A	1204	FJY	C20-C18-C17	3.23	133.55	125.39
3	A	1204	FJY	C8-C9-N1	-3.20	120.11	123.23
3	A	1204	FJY	C18-C19-N2	2.99	111.70	109.76
3	A	1204	FJY	C14-N3-C15	2.84	121.77	116.85
3	A	1204	FJY	C5-C4-C3	-2.67	120.28	123.23
3	A	1204	FJY	C23-C19-C18	-2.59	118.92	122.00
3	A	1204	FJY	C9-N1-C2	2.46	122.27	117.27
3	A	1204	FJY	C1-C2-N1	-2.39	120.27	122.81
3	A	1204	FJY	C25-C17-C18	-2.13	107.16	110.98
3	A	1204	FJY	C17-C18-C19	-2.12	106.20	110.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	FJY	C15-C10-C9-N1

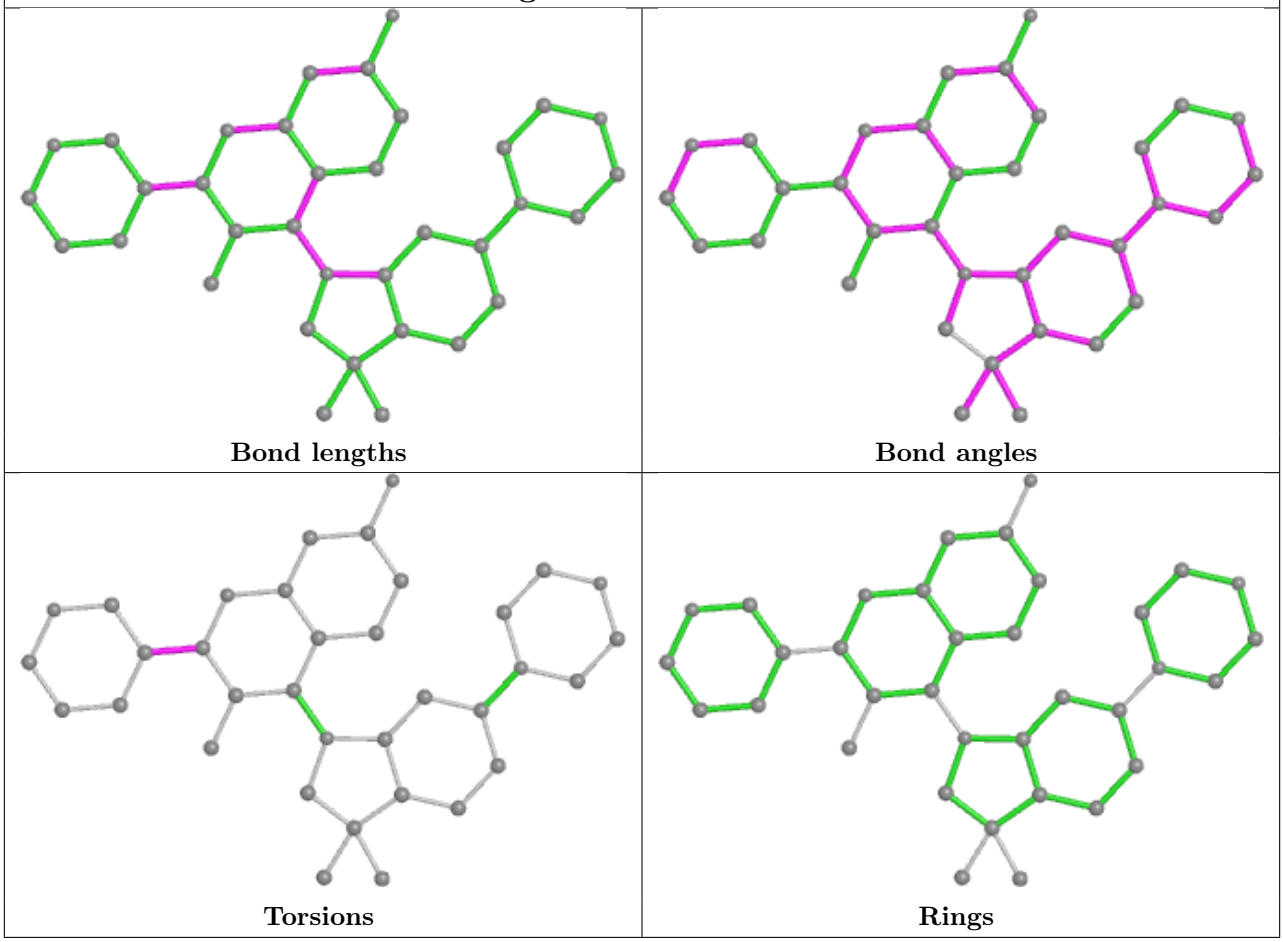
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1204	FJY	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FJY A 1204



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	839/960 (87%)	0.05	47 (5%) 24 20	53, 97, 155, 204	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1000	LYS	5.3
1	A	999	GLY	5.2
1	A	270	PHE	4.9
1	A	895	THR	4.8
1	A	457	LYS	4.7
1	A	532	HIS	4.7
1	A	351	THR	4.3
1	A	998	SER	4.2
1	A	936	CYS	4.1
1	A	352	VAL	3.6
1	A	899	THR	3.4
1	A	1041	GLN	3.4
1	A	545	ALA	3.3
1	A	320	LYS	3.2
1	A	898	ASN	3.2
1	A	531	LYS	3.1
1	A	234	LYS	3.0
1	A	217	ASN	2.9
1	A	144	SER	2.9
1	A	145	GLU	2.9
1	A	945	GLY	2.9
1	A	309	THR	2.8
1	A	216	ALA	2.8
1	A	458	VAL	2.7
1	A	986	VAL	2.7
1	A	310	PRO	2.5
1	A	894	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	995	MET	2.5
1	A	533	GLN	2.5
1	A	1044	SER	2.4
1	A	766	GLN	2.4
1	A	355	TRP	2.3
1	A	215	ILE	2.3
1	A	511	GLU	2.3
1	A	530	PRO	2.3
1	A	916	PRO	2.3
1	A	148	GLN	2.3
1	A	932	CYS	2.3
1	A	211	LEU	2.3
1	A	985	PHE	2.2
1	A	897	GLY	2.2
1	A	307	LEU	2.2
1	A	319	ARG	2.2
1	A	152	ARG	2.1
1	A	488	SER	2.1
1	A	1042	LEU	2.0
1	A	526	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FJY	A	1204	35/35	0.89	0.31	73,116,127,129	0
2	SO4	A	1201	5/5	0.92	0.20	116,121,131,144	0
2	SO4	A	1203	5/5	0.93	0.19	97,101,108,113	0

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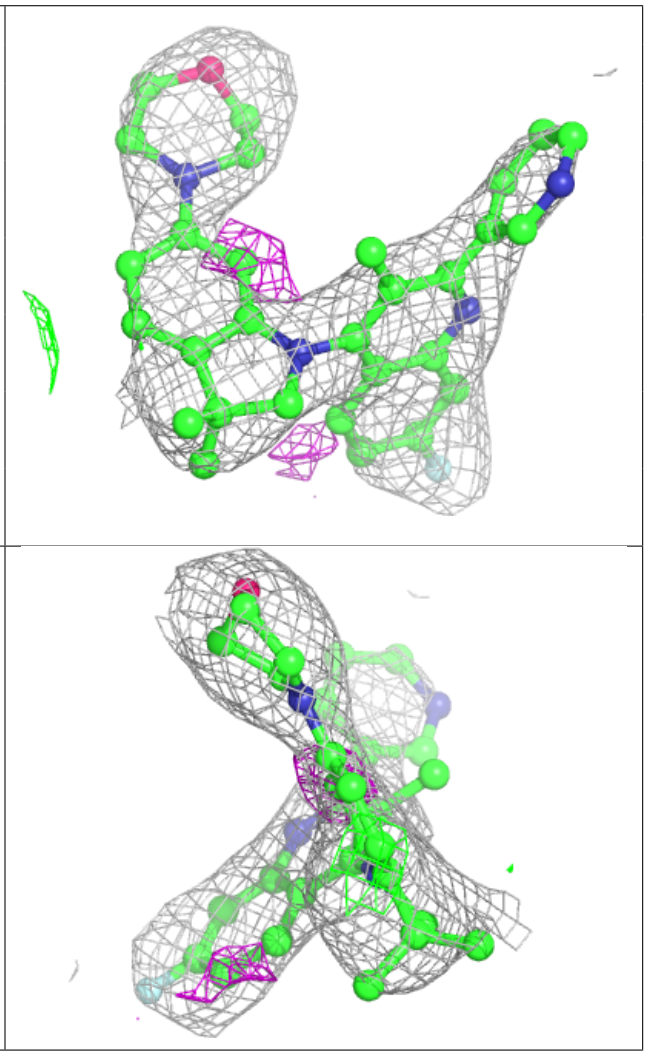
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	1202	5/5	0.97	0.11	84,89,97,106	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FJY A 1204:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.